DSSTox Field Definition File:

EPA Integrated Risk Information System (IRIS) Toxicity Review Data (IRISTR)

(last updated 19 February 2008)

Description: Information in this file is intended to provide a minimum level of annotation to the DSSTox SDF (Structure Data Format) file created for the EPA IRIS Toxicity Review Data (IRISTR) file constructed from information extracted from the EPA IRIS Source website. For further explanation of Source-specific fields, a user should consult the Source website (http://www.epa.gov/iris/). Additional information is provided on the DSSTox IRISTR SDF Download Page http://www.epa.gov/ncct/dsstox/sdf_iristr.html. A number of modifications in fields (and allowable entries) were made to the original information extracted from the EPA IRIS Source website to improve consistency in notations and facilitate use of the DSSTox SDF files in relational searching applications. All modifications are documented in the ***Comments*** section of the table below. Most of the field definitions below were extracted from either the IRIS Glossary (http://www.epa.gov/iris/gloss8.htm) or from Guidance Documents or other reference materials on the IRIS Source Website. Wherever possible, we refer the user to the relevant IRIS webpage.

Most of the IRISTR Source-Specific Fields were directly extracted from the EPA IRIS Source Website in Oct 2006 using the "Multiple Substance Report" page (left side-bar link on the IRIS Home page): all chemical substances in the "Select Multiple Substances" window were selected; and all 5 "types of data to compare", or toxicity review areas, were selected (Oral RfDs, Inhalation RfCs, Weight of Evidence Characterizations, Oral Slope Factors/Drinking Water Risks, Air Unit Risks). Clicking on "Generate a Web Report" generated several html tables, one corresponding to each toxicity review area, which were subsequently transferred to a single Excel data table. These data underwent extensive cleaning and modification to standardize, simplify, and create more consistent text entries and notations. Changes included: conversion of all quantitative information fields (Oral RfDs, Inhalation RfCs, etc) to pure numeric form; conversion of mg unit fields to mmol unit fields; addition of integer "count" fields for each toxicity review assessment area (to enable quick counting and extraction of the subset of substances evaluated in each of the 5 toxicity review areas); elimination of abbreviations and footnotes; and some editing and standardization of "Critical Effects" and "Precursor Effect/Tumor Type" field entries to be more consistent throughout the file. The original IRIS field (column header) names and any modifications to the original IRIS field data are documented in the ***Comments*** column below. Fields not obtained from this IRIS Web Report, but added by us to the DSSTox file are explicitly noted. A table of IRIS toxicity review categories and column headers, and corresponding DSSTox IRISTR fields is also provided in the IRISTR_LogFile, available on the DSSTox IRISTR SDF Download Page http://www.epa.gov/ncct/dsstox/sdf_iristr.html.

Description of ***DSSTox Standard Chemical Fields*** can be found in the Central Field Definition Table located at:
http://www.epa.gov/ncct/dsstox/CentralFieldDef.html

The first section of the Table below lists the ***DSSTox Standard Toxicity Fields*** employed for this database, followed by the ***IRISTR Source-Specific Fields*** containing the toxicity assessment information particular to IRISTR. The ***Field Type*** indicates the type of the field, such as numeric, integer, defined text, memo, etc. All ***Units*** and ***Descriptions*** are extracted from Source reference materials unless otherwise noted. ***Allowable Entries*** lists allowed field entries occurring in IRISTR, separated by slashes for exclusive entries (i.e., cannot occur with another entry) and semicolons or spaces for non-exclusive entries (i.e., can occur with other values). These are defined and explained in the ***Description*** section.

Source Website: http://www.epa.gov/iris/

Source Contact: For technical questions about the scientific information content in IRIS, contact the US EPA Risk Information Hotline: phone (202)566-1676; fax (202)566-1749; or email: hotline.iris@epa.gov

SDF Usage Notes:
Each DSSTox SDF file contains a single **STRUCTURE** field. For each chemical record, the **STRUCTURE** field entry directly corresponds to the content of the **STRUCTURE_...** fields. The **STRUCTURE_Shown** field documents the relationship between what is displayed in the **STRUCTURE** field and the actual tested chemical substance, i.e. **TestSubstance_...** fields, with the latter corresponding directly to the toxicity data field entries. Commercial chemical relational database (CRD) applications may automatically insert one or more structure identifier fields upon import or export of an SDF file (e.g., Formula, FW or Mol_ID), fields that

may augment or duplicate one or more of the DSSTox Standard Chemical Fields. Users are cautioned that fields containing null values in the first record of the SDF will be reordered upon import into most applications; for this reason, the word "blank" has been inserted into null fields in Record 1 of DSSTox SDF files and can be deleted after SDF import. Users are additionally cautioned that some fields (**STRUCTURE_SMILES** and **STRUCTURE_InChI**, in particular) may exceed the 200 character limit specified in the MDL CTFiles SDF standard (see http://www.epa.gov/ncct/dsstox/MoreonSDF.html), and that some CRD applications may insert a line break or truncate these fields upon SDF import or export. Finally, CRD application-specific molecular header information in the SDF file is deleted in the final DSSTox SDF files; users running CRD applications requiring a unique molecule header upon import of the SDF can specify either **DSSTox_RID** or the **DSSTox_FileID** be used. Upon SDF import, **DSSTox_CID** can be used to identify and manage chemical structure duplicates and **DSSTox_Generic_SID** can be used to identify common Test Substances across and within DSSTox files (similar to CASRN-substance, but available for all DSSTox substances and further distinguishes among different purity/grade substances).

As an MS Word document, the following table is best viewed onscreen using either Normal or Web Layout View in Landscape page orientation.

Field Name *(no spaces)*	***Field Type***	***Units***	***Allowable Entries***	***Description***	***Comments***
			DSSTox Standard Toxicity Fields		
Study Type	defined text		Human Health Exposure Toxicity Review for Risk Assessment	Field is used to label all records in the database, generally with the same entry, and is designed to facilitate record identification for cross-database structure searching. Field entry refers to the main type of toxicity study for which data is represented in the database.	Field names and content are being coordinated with the public ToxML standardization effort.
Endpoint	defined text		cancer; acute; short-term; sub-chronic; chronic; developmental	Field is used to label all records in the database, generally with the same entry, and is designed to facilitate record identification for cross-database structure searching. Field entry refers to the type of toxicity measure represented within the database.	Field names and content are being coordinated with the public ToxML standardization effort.
Species	defined text		rodent; human; dog; rabbit	Field is used to label all records in the database, generally with the same entry, and is designed to facilitate record identification for cross-database structure searching. Field entry refers to the species of animal(s) listed in the data record and used in the toxicity study or studies.	Field names and content are being coordinated with the public ToxML standardization effort. Study species varies across IRIS documents, with only occasional mention of non-rodent test species. Users should consult IRIS Summary for study details.
			IRISTR Source-Specific Fields		
Oral_RfD_ Assessed	integer		1/ 0/	Value indicates whether oral exposure Reference Dose (RfD) was assessed (1) or not (0) for this substance. See **Oral_RfD_mg_per_kg_day** for definition of oral reference dose.	Counter field added to DSSTox file. Corresponds to content under IRIS Multiple Substance Report search results category: "Oral RfDs".
Oral_RfD_CriticalEffects	text		abnormal blood pigment; argyria;	Critical Effects are defined as the first adverse effect, or its known precursor, that occurs to the most sensitive species as the dose rate of an agent increases. Listed here are critical effects pertaining to oral exposures that are used to compute oral reference doses (RfD) for the	No standard vocabulary or ontology was used here. However, original IRIS entries were modified in some cases

			ataxia; atrophy; autoimmune effects; blood pressure changes; body weight changes; cataract formation; cholinesterase (ChE) inhibition; decreased body weight; degeneration kidney tubules; delayed neurotoxicity; liver cell changes-females liver histopathology; … Information reviewed but value not estimated; refer to IRIS Summary./ Not assessed under the IRIS program./	substance. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). If no critical effects are reported, entry is either: "Information reviewed but value not estimated; refer to IRIS Summary." or "Not assessed under the IRIS program."	to adopt consistent notation throughout this data file, e.g. "reduced body weight" was changed to "decreased body weight" in all cases. Future versions may attempt to reconcile field entries with ToxML standard terminology. Corresponds to content under IRIS Multiple Substance Report search results category: "Oral RfDs". Original IRIS column header: "Critical Effects".
Oral_RfD_mg_per_kg_day	numeric	mg/kg-bw/day	#/ *blank*	Oral Reference Dose (RfD) is based on the assumption that thresholds exist for certain toxic effects such as cellular necrosis. It is based on oral exposure and expressed in units of mg/kg-day. It is an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a NOAEL (no observed adverse effect level), LOAEL (lowest observed adverse effect level), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. Generally used in EPA's noncancer health assessments. [Durations include acute, short-term, subchronic, and chronic and are defined individually in the IRIS glossary at http://www.epa.gov/iris/gloss8.htm]. Dose units are mg/kg-(body weight) per day. For more information, see http://www.epa.gov/iris/rfd.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no value computed.	Original IRIS values converted to pure numeric form for a single reported oral RfD. In a few instances, multiple reported values of the oral RfD for a single substance or footnotes have been incorporated into the field **Oral_RfD_Notes**. Corresponds to content under IRIS Multiple Substance Report search results category: "Oral RfDs". Original IRIS column header: "Oral RfD".
Oral_RfD_mmol_per_kg_day	numeric	mmol/kg-bw/day	#/ *blank*	**Oral_RfD_mg_per_kg_day** value converted to molar units in cases where test substance is not a mixture of different molecular weight substances, based on formula: **Oral_RfD_mg_per_kg_day**/**STRUCTURE_MolecularWeight**; molar	Field added to DSSTox file. Molar values are more appropriate for molecule to molecule activity comparisons,

				units should be used for any structure-activity relationship comparisons. "blank" or null entry indicates no oral RfD value computed or substance is a mixture not suitable for molar unit conversion.	such as in structure-activity relationships.
Oral_RfD_Notes	memo		*Text/* *blank*	Point of Departure is the dose-response point that marks the beginning of a low-dose extrapolation. This point can be the lower bound on dose for an estimated incidence or a change in response level from a dose-response model (BMD - Benchmark dose), or a NOAEL (no observed adverse effect level) or LOAEL (lowest observed adverse effect level) for an observed incidence, or change in level of response. Field also includes details in cases where multiple Oral RfDs are reported. For more information, see http://www.epa.gov/iris/rfd.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no oral RfD value computed.	Corresponds to content under IRIS Multiple Substance Report search results category: "Oral RfDs". Original IRIS column header: "Point of Departure(s)". Footnotes or multiple Oral RfDs from the IRIS "Oral RfD" column were also moved to this text Note field. Abbreviations are expanded in DSSTox field entries.
Oral_RfD_Confidence	defined text		High/ Medium-High Medium/ Low-Medium/ Low/ *blank*	Confidence in Oral RfD is based on several factors, including availability of epidemiology and other supporting data, quality of studies, magnitude of effect, etc. For more information, see http://www.epa.gov/iris/rfd.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no oral RfD value computed.	Corresponds to content under IRIS Multiple Substance Report search results category: "Oral RfDs". Original IRIS column header: "Overall Confidence".
Inhalation_RfC_Assessed	integer		1/ 0/	Value indicates whether inhalation exposure Reference Dose was assessed (1) or not (0) for this substance. See **Inhalation_RfC_mg_per_m3** for definition of inhalation reference dose.	Counter field added to DSSTox file. Corresponds to content under IRIS Multiple Substance Report search results category: "Inhalation RfCs".
Inhalation_RfC_CriticalEffects	text		altered nasal turbinates; altered red blood cell (RBC) count; beryllium sensitization; bronchiolar fibrosis; cerebellar lesions; cholinesterase (ChE) inhibition brain; chronic lung function decline; CNS effects; … Information reviewed but value not estimated; refer to	Critical Effects are defined as the first adverse effect, or its known precursor, that occurs to the most sensitive species as the dose rate of an agent increases. Listed here are critical effects pertaining to inhalation exposures that are used to compute inhalation reference concentrations (RfC) for the substance. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). If no critical effects are reported, entry is either: "Information reviewed but value not estimated; refer to IRIS Summary." or "Not assessed under the IRIS program."	No standard vocabulary or ontology was used here. However, original IRIS entries were modified in some cases to adopt consistent notation throughout this data file, e.g. "reduced body weight" was changed to "decreased body weight" in all cases. Future versions may attempt to reconcile field entries with ToxML standard terminology. Corresponds to content under IRIS Multiple Substance Report search results category: "Inhalation RfCs". Original IRIS column header: "Critical Effects".

			IRIS Summary./ Not assessed under the IRIS program./		
Inhalation_RfC_mg_per_m3	numeric	mg/m3	#/ *blank*	Inhalation Reference Concentration (RfC) is based on the assumption that thresholds exist for certain toxic effects such as cellular necrosis. It is based on inhalation exposure and expressed in units of mg/m3 air volume. It is an estimate (with uncertainty spanning perhaps an order of magnitude) of a continuous inhalation exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a NOAEL (no observed adverse effect level), LOAEL (lowest observed adverse effect level), or benchmark concentration (BMC), with uncertainty factors generally applied to reflect limitations of the data used. Generally used in EPA's noncancer health assessments. [Durations include acute, short-term, subchronic, and chronic and are defined individually in the IRIS glossary at http://www.epa.gov/iris/gloss8.htm Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no inhalation RfC value computed.	Original IRIS values converted to pure numeric form for a single reported inhalation RfC. In a few instances, multiple reported values of the inhalation RfC for a single substance or footnotes have been incorporated into the field **Inhalation_RfC_Notes**. Corresponds to content under IRIS Multiple Substance Report search results category: "Inhalation RfCs". Original IRIS column header: "Inhalation RfC".
Inhalation_RfC_mmol_per_m3	numeric	mmol/ m3	#/ *blank*	**Inhalation_RfC_mg_per_m3** value converted to molar units in cases where test substance is not a mixture of different molecular weight substances, based on formula: **Inhalation_RfC_mg_per_m3/STRUCTURE_MolecularWeight**; molar units should be used for any structure-activity relationship comparisons. "blank" or null entry indicates no inhalation RfC value computed or substance is a mixture not suitable for molar unit conversion.	Field added to DSSTox file. Molar values are more appropriate for molecule to molecule activity comparisons, such as in structure-activity relationships.
Inhalation_RfC_Notes	memo		*Text*	Point of Departure is the dose-response point that marks the beginning of a low-dose extrapolation. This point can be the lower bound on dose for an estimated incidence or a change in response level from a dose-response model (BMD - Benchmark dose), or a NOAEL (no observed adverse effect level) or LOAEL (lowest observed adverse effect level) for an observed incidence, or change in level of response. For more information, see http://www.epa.gov/iris/rfd.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no inhalation RfC value computed.	Corresponds to content under IRIS Multiple Substance Report search results category: "Inhalation RfCs". Original IRIS column header: "Point of Departure(s)". Footnotes or multiple Inhalation RfCs from the IRIS "Inhalation RfC" column were also moved to this text Note field. Abbreviations are expanded in DSSTox field entries.
Inhalation_RfC_Confidence	defined text		High/ Medium-High Medium/ Low-Medium/ Low/ *blank*	Confidence in Inhalation RfC is based on several factors, including availability of epidemiology and other supporting data, quality of studies, magnitude of effect, etc. For more information, see http://www.epa.gov/iris/rfd.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no inhalation RfC value computed.	Corresponds to content under IRIS Multiple Substance Report search results category: "Inhalation RfCs". Original IRIS column header: "Overall Confidence".
WtOfEvidence_Cancer_Assessed	integer		#	Value indicates whether Weight of Evidence for Carcinogenicity was assessed (1) or not (0) for this substance. See	Counter field added to DSSTox file.

				WtOfEvidence_Cancer_Narrative for description of approach.	Corresponds to content under IRIS Multiple Substance Report search results category: “Weight of Evidence Characterizations”.
WtOfEvidence_Cancer_Concern	defined text		High/ Medium-High Medium/ Low-Medium/ Low/ Inadequate evidence/ *blank*	Weight-of-Evidence (WOE) for carcinogenicity Concern Level is assigned based on the type and sufficiency of evidence available for human risk and takes one of the following values: High, Medium-High, Medium, Low-Medium, Low, Inadequate evidence. See **WtOfEvidence_Cancer_Narrative** for description of approach and pgs 19-21 of http://www.epa.gov/ncea/raf/car2sab/guidelines_1986.pdf). Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no assessment performed.	Corresponds to content under IRIS Multiple Substance Report search results category: “Weight of Evidence Characterizations”. Field added to DSSTox file based on level of concern table provided in Cancer Guidelines corresponding to the Guideline Categories (A-D).
WtOfEvidence_1986GuidelineCategories	defined text		A; Human Carcinogen/ B1; Probable human carcinogen - based on limited evidence of carcinogenicity in humans/ B2; Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals/ C; Possible human carcinogen/ D; Not classifiable as to human carcinogenicity/ E; Evidence of non-carcinogenicity for humans/ Information reviewed but value not estimated - refer to IRIS Summary./ Not assessed under the IRIS program./	Based on the EPA' 1986 Cancer Risk Assessment Guidelines, the Weight of Evidence determination assigns the substance to one of the following categories: Group A - Human Carcinogen; Group B1 - Probable human carcinogen based on limited evidence of carcinogenicity in humans; Group B2 - Probable human carcinogen based on sufficient evidence of carcinogenicity in animals; Group C - Possible human carcinogen; Group D - Not classifiable as to human carcinogenicity; Group E - Evidence of non-carcinogenicity for humans; Information reviewed but value not estimated - refer to IRIS Summary; Not applicable - this substance was not assessed using the 1986 cancer guidelines (US EPA 1986); Not assessed under the IRIS program. Note: The majority of IRIS Cancer Risk assessments are based on the 1986 guidelines. However, updates to these guidelines were published in 1996, 1999 and 2005 (see http://www.epa.gov/iris/backgr-d.htm), and superseded the earlier 1986 guidelines. Current IRIS assessments use the 2005 Guidelines for Carcinogen Assessment: http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=116283) with revised categories: “Carcinogenic to Humans”, “Likely to be Carcinogenic to Humans”, “Suggestive Evidence of Carcinogenic Potential”, “Inadequate Information to Assess Carcinogenic Potential”, “Not Likely to be Carcinogenic to Humans”. Revised or updated guidelines and cancer risk characterizations, if applicable, are provided in the field “**WtOfEvidence_Cancer_Narrative**”.	Corresponds to content under IRIS Multiple Substance Report search results category: “Weight of Evidence Characterizations”. Original IRIS column header: “WOE 86 Guidelines”. Abbreviations for Guideline Categories (A-D) are expanded in DSSTox field entries.

			Not applicable. This substance was not assessed using the 1986 cancer guidelines (US EPA 1986)./		
WtOfEvidence_UpdatedGuidelineUsed	defined text		Updated US EPA [1996, 1999, or 2005] Guidelines used; see WtOfEvidence_Cancer_Narrative. *blank*	Field entry indicates when updated (newer than 1986) EPA Guidelines were used in the Weight of Evidence determination for cancer. Entry makes reference to 1996, 1999, or 2005 updated EPA Guidelines, with additional details provided in the **WtOfEvidence_Cancer_Narrative** field. "blank" or null entry indicates no updated Guidelines were used.	Field added to DSSTox file to inform users of instances of where updated EPA Guidelines newer than 1986 usage in IRIS assessments.
WtOfEvidence_Cancer_Narrative	memo		*Text/* *blank*	Weight-of-Evidence (WOE) for Carcinogenicity is a system used by the U.S. EPA for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. Under EPA's 1986 risk assessment guidelines the WOE was described by categories "A through E", Group A for known human carcinogens through Group E for agents with evidence of noncarcinogenicity (see WtOfEvidence_1986GuidelineCategories, and http://www.epa.gov/ncea/raf/car2sab/guidelines_1986.pdf). Revised guidelines published in 1996, 1999, and 2005 have modified these cancer risk characterizations. The approach outlined in EPA's guidelines for carcinogen risk assessment (2005) considers all scientific information in determining whether and under what conditions an agent may cause cancer in humans, and provides a narrative approach to characterize carcinogenicity rather than categories. Five standard weight-of-evidence descriptors are used as part of the narrative and overall Concern Level is indicated based on all considered information (see **WtOfEvidence_Cancer_Concern**). Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no assessment performed.	Corresponds to content under IRIS Multiple Substance Report search results category: "Weight of Evidence Characterizations". Original IRIS column header: "WOE 86 Narrative".
DrinkingWater_OralSlope_Assessed	integer		*#/*	Value indicates whether drinking water oral exposure Slope Factor was assessed (1) or not (0) for this substance. See **DrinkingWater_OralSlopeFactor_mg_per_kg_day** for definition of drinking water Oral Slope Factor.	Counter field added to DSSTox file. Corresponds to content under IRIS Multiple Substance. Report search results category: "Oral Slope Factors/Drinking Water Unit Risks".
DrinkingWater_PrecursorEffect_TumorType	text		abdominal cavity sarcomas; brain and spinal cord astrocytomas; Zymbal gland carcinomas; stomach papillomas; stomach	Listing of the pre-carcinogenic cellular abnormality and/or tumor type that factor into the determination of the Oral Slope Factor and Unit Risk. Precursor effects in specified organ/tissues include, e.g., adenomas, neoplastic nodules, carcinomas, astrocytomas, papillomas. Tumors are indicated by listing of organ or tissue without additional qualifiers, e.g., bladder, liver, kidney, etc. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). If no precursor effects are reported, entry is either:	No standard vocabulary or ontology was used here. However, original IRIS entries were modified in some cases to adopt consistent notation throughout this data file. Future versions may attempt to reconcile field entries with ToxML standard terminology.

			carcinomas; CNS; mammary gland; thyroid gland; uterus; pelvis carcinomas; urinary bladder papillomas; thyroid adenomas; thyroid carcinomas; forestomach papillomas; forestomach carcinomas forestomach; leukemia; hemangiosarcomas; … Information reviewed but value not estimated; refer to IRIS Summary./ Not assessed under the IRIS program./	"Information reviewed but value not estimated; refer to IRIS Summary." or "Not assessed under the IRIS program."	Corresponds to content under IRIS Multiple Substance Report search results category: "Oral Slope Factors/Drinking Water Unit Risks". Original IRIS column header: "Precursor Effect/Tumor Type".
DrinkingWater_OralSlopeFactor_mg_per_kg_day	numeric	mg/kg-bw/day	#/ *blank*	Slope Factor refers to an upper bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100. Values reported here are computed from oral drinking water exposure data and expressed in units of mg/kg-(body weight) per day. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no oral slope factor determined.	Field values converted to pure numeric form for a single reported oral slope factor. In a few instances, multiple reported values of the oral slope factor for a single substance or footnotes have been incorporated into the field **DrinkingWater_ExtrapolationMethod_Notes**. Corresponds to content under IRIS Multiple Substance Report search results category: "Oral Slope Factors/Drinking Water Unit Risks". Original IRIS column header: "Oral Slope Factors".
DrinkingWater_OralSlopeFactor_mmol	numeric	mmol/kg-	#/ *blank*	**DrinkingWater_OralSlopeFactor_mg_per_kg_day** value converted to molar units in cases where test substance is not a mixture of	Field added to DSSTox file. Molar values are more

_per_kg_day		bw/day		different molecular weight substances, based on formula: **DrinkingWater_OralSlopeFactor_mg_per_kg_day/STRUCTURE_MolecularWeight**; molar units should be used for any structure-activity relationship comparisons. "blank" or null entry indicates no oral slope factor determined or substance is a mixture not suitable for molar unit conversion.	appropriate for molecule to molecule activity comparisons, such as in structure-activity relationships.
DrinkingWater_ExtrapolationMethod_Notes	memo		*Text/* *blank*	Lists extrapolation method used to compute Oral Slope Factor and additional details of this calculation. May also list any additional Oral Slope Factors and Unit Risks for this substance, indication of extra risk, and units. Extrapolation methods include, e.g., linearized multi-stage procedure, one-hit with time factor, multistage model with Benchmark Dose modeling, etc. "blank" or null entry indicates no oral slope factor determined. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no oral slope factor determined.	Corresponds to content under IRIS Multiple Substance Report search results category: "Oral Slope Factors/Drinking Water Unit Risks". Original IRIS column header: "Extrapolation Method". Footnotes or multiple Oral Slope Factors or Unit Risks from the IRIS ""Oral Slope Factors" or "Drinking Water Unit Risks" columns were also moved to this text Note field. Abbreviations are expanded in DSSTox field entries.
DrinkingWater_UnitRisk_microg_per_L	numeric	microg/L	#/ *blank*	Unit Risk is defined as the upper-bound excess lifetime cancer risk estimated to result from continuous exposure to an agent at a concentration of 1 µg/L in water, or 1 µg/m3 in air. The interpretation of unit risk would be as follows: if unit risk = 2 x 10-6 per microg/L, 2 excess cancer cases (upper bound estimate) are expected to develop per 1,000,000 people if exposed daily for a lifetime to 1 microg of the chemical in 1 liter of drinking water. Units are microgram/L. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no unit risk determined.	Corresponds to content under IRIS Multiple Substance Report search results category: "Oral Slope Factors/Drinking Water Unit Risks". Original IRIS column header: "Drinking Water Unit Risks".
DrinkingWater_UnitRisk_micromol_per_L	numeric	micromol/L	#/ *blank*	**DrinkingWater_UnitRisk_microg_per_L** value converted to molar units in cases where test substance is not a mixture of different molecular weight substances, based on formula: **DrinkingWater_UnitRisk_microg_per_L/STRUCTURE_MolecularWeight**; molar units should be used for any structure-activity relationship comparisons. "blank" or null entry indicates no unit risk determined or substance is a mixture not suitable for molar unit conversion.	Field added to DSSTox file. Molar values are more appropriate for molecule to molecule activity comparisons, such as in structure-activity relationships.
DrinkingWater_StudyRoute	defined text		diet; drinking water; gavage; inhalation; occupational exposure; oral; corn oil; sesame oil;	Route of administration of study used to estimate Drinking Water exposure route Oral Slope Factor and Unit Risk. Possibilities include: diet, drinking water, gavage, inhalation, occupational exposure, oral. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no study results reported. NTP = NIH National Toxicology Program NCA = National Cancer Association	Corresponds to content under IRIS Multiple Substance Report search results category: "Oral Slope Factors/Drinking Water Unit Risks". Original IRIS column header: "Study Route".

			salad oil/ (NTP, NCA) *blank*		
Inhalation_UnitRisk_Assessed	integer		#	Value indicates whether inhalation exposure Unit Risk was assessed (1) or not (0) for this substance. See **Inhalation_UnitRisk_microg_per_m3** for description of inhalation exposure Unit Risk values.	Counter field added to DSSTox file. Corresponds to content under IRIS Multiple Substance Report search results category: “Air Unit Risks”. Older IRIS assessments use the term “Air”, whereas newer assessments substitute the equivalent term “Inhalation”.
Inhalation_PrecursorEffect_TumorType	text		abdominal cavity sarcomas; bladder; esophagus; bronchioalveolar adenoma; CNS; mammary and thyroid glands; uterus; oral cavity (combined); hemangiosarcomas; … Information reviewed but value not estimated; refer to IRIS Summary./ Not assessed under the IRIS program./	Listing of the pre-carcinogenic cellular abnormality and/or tumor type that factor into the determination of the Air Unit Risk. Precursor effects in specified organ/tissues include, e.g., adenomas, neoplastic nodules, carcinomas, astrocytomas, papillomas. Tumors are indicated by listing of organ or tissue without additional qualifiers, e.g., bladder, liver, kidney, etc. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). If no precursor effects are reported, entry is either: "Information reviewed but value not estimated; refer to IRIS Summary." or "Not assessed under the IRIS program.”	No standard vocabulary or ontology was used here. However, original IRIS entries were modified in some cases to adopt consistent notation throughout this data file. Future versions may attempt to reconcile field entries with ToxML standard terminology. Corresponds to content under IRIS Multiple Substance Report search results category: “Air Unit Risks”. Original IRIS column header: “Precursor Effect/Tumor type”. Older IRIS assessments use the term “Air”, whereas newer assessments substitute the equivalent term “Inhalation”.
Inhalation_UnitRisk_microg_per_m3	numeric	microg/m3	#/ *blank*	Unit Risk is defined as the upper-bound excess lifetime cancer risk estimated to result from continuous exposure to an agent at a concentration of 1 µg/L in water, or 1 µg/m3 in air. The interpretation of unit risk would be as follows: if unit risk = 2 x 10-6 per microg/L, 2 excess cancer cases (upper bound estimate) are expected to develop per 1,000,000 people if exposed daily for a lifetime to 1 microg of the chemical in 1 liter of drinking water. Units are microgram/cubicmeter volume of air. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no unit risk determined.	Corresponds to content under IRIS Multiple Substance Report search results category: “Air Unit Risks”. Original IRIS column header: “Air Unit Risks”. Older IRIS assessments use the term “Air”, whereas newer assessments substitute the equivalent term “Inhalation”.
Inhalation_UnitRisk	numeric	microm	#/	**Inhalation_UnitRisk_microg_per_m3** value converted to molar units	Field added to DSSTox file.

_micromol_per_m3		ol/m3	*blank*	in cases where test substance is not a mixture of different molecular weight substances, based on formula: **Inhalation _UnitRisk_microg_per_m3** / **STRUCTURE_MolecularWeight**; molar units should be used for any structure-activity relationship comparisons. "blank" or null entry indicates no unit risk determined or substance is a mixture not suitable for molar unit conversion.	Molar values are more appropriate for molecule to molecule activity comparisons, such as in structure-activity relationships.
Inhalation_StudyRoute	defined text		diet; drinking water; gavage; inhalation; occupational exposure; oral; gavage followed by diet; gavage in corn oil/ *blank*	Route of administration of study used to estimate Inhalation exposure route Oral Slope Factor and Unit Risk. Possibilities include: diet, drinking water, gavage, inhalation, occupational exposure, oral. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no study results reported.	Corresponds to content under IRIS Multiple Substance Report search results category: "Air Unit Risks". Original IRIS column header: "Study Route". Older IRIS assessments use the term "Air", whereas newer assessments substitute the equivalent term "Inhalation".
Inhalation_ExtrapolationMethod_Notes	memo		*Text*	Lists extrapolation method used to compute Air (Inhalation) Unit Risk and additional details of this calculation. May also list any additional Unit Risks for a substance, indication of extra risk, and units. Extrapolation methods include, e.g., linearized multi-stage procedure, one-hit with time factor, multistage model with Benchmark Dose modeling, etc. For more information, see: http://www.epa.gov/iris/carcino.htm. Refer to the IRIS Summary for more details on a particular chemical assessment (can be accessed from the QuickView **Website_URL**). "blank" or null entry indicates no unit risk determined.	Corresponds to content under IRIS Multiple Substance Report search results category: "Air Unit Risks". Original IRIS column header: "Extrapolation Method". Older IRIS assessments use the term "Air", whereas newer assessments substitute the equivalent term "Inhalation".
TotalAssessments	integer		#	Sum of indicator values (0,1) for assessments in all 5 toxicity review areas (Oral RfDs, Inhalation RfCs, Weight of Evidence Characterizations, Oral Slope Factors/Drinking Water Unit Risks, Air Unit Risks), with total ranging from 0-5 providing a rough indication of the amount of study data available for a given substance.	Counter field added to DSSTox file. Corresponds to content under IRIS Multiple Substance Report search results for all 5 listed search categories.
Note_IRISTR	memo		*Text*	Field used to provide supplementary Source-specific information pertaining to the chemical and toxicity fields.	Any discrepancies in IRIS CAS vs. DSSTox CAS or test substance description are provided here. See IRISTR Log File for more details.
ChemicalPage_URL	URL		*Text*	Internet URL website address linking to external web page providing chemical-specific data or content. ChemicalPage_URL was checked at time of DSSTox data file publication. Please send DSSTox Error Report if website URL address no longer works or is changed.	URLs are provided for the IRIS "Quick View" web pages. Links to the IRIS Summary documents are easily accessed from these pages. URLs were extracted at the time of initial DSSTox file

					creation (Oct 2006). Efforts will be made to coordinate IRIS Website updates affecting data content or URL addresses with the content of this DSSTox file.